

# ANN and Fuzzy c-Means Applied to Environmental Pollution Prediction

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**Abstract**—Salamanca, situated in center of Mexico is among the cities which suffer most from the air pollution in Mexico. The vehicular park and the industry, as well as orography and climatic characteristics have propitiated the increment in pollutant concentration of Sulphur Dioxide ( $SO_2$ ). In this work, a Multilayer Perceptron Neural Network has been used to make the prediction of an hour ahead of pollutant concentration. A database used to train the Neural Network corresponds to historical time series of meteorological variables and air pollutant concentrations of  $SO_2$ . Before the prediction, Fuzzy c-Means and K-means clustering algorithms have been implemented in order to find relationship among pollutant and meteorological variables. Our experiments with the proposed system show the importance of this set of meteorological variables on the prediction of  $SO_2$  pollutant concentrations and the neural network efficiency. The performance estimation is determined using the Root Mean Square Error (RMSE) and Mean Absolute Error (MAE). The results showed that the information obtained in the clustering step allows a prediction of an hour ahead, with data from past 2 hours.

## I. INTRODUCTION

Air pollution is contamination of environment by any chemical, physical or biological agent that modifies the natural characteristics of the atmosphere [1]. Smog hanging over cities is the most familiar and obvious form of air pollution. Generally any substance that people introduce into the atmosphere that has damaging effects on living things and the environment is considered air pollution, and these contribute to global warming. Pollutants of major public health concern include Particulate Matter (PM), carbon monoxide (CO), ozone ( $O_3$ ), nitrogen dioxide ( $NO_2$ ) and sulfur dioxide ( $SO_2$ ).

Clean air is considered to be a basic requirement of human health and well-being. However, air pollution continues to pose a significant threat to health worldwide. According to a WHO assessment of the burden of disease due to air pollution, more than 2 million premature deaths each year can be attributed to the effects of urban outdoor air pollution and indoor air pollution (caused by the burning of solid fuels). More than half of this disease burden is borne by the populations of developing countries [2]. The inhalation of air polluted with particulate matter or irritant gases such as Nitrogen oxides and Sulphur Dioxide are associated with

both short-term and long-term health effects, most of which impact on the respiratory and cardiovascular systems [3].

The air quality in cities varies depending on the industrialization, population and traffic density; and meteorological and topographical properties of the region [4], [5]. Especially in industrialized cities, the pollutants exhausted, emitted and discharged by the industrial foundations have the most significant effect in environmental pollution. Among the meteorological parameters, wind speed can be effective in decreasing pollutant concentration. Normally pollutants rise or flow away from their sources without building up to unsafe levels. Wind patterns, clouds, rain, and temperature can affect how quickly pollutants move away from an area. Weather patterns that can trap air pollution in valleys or move it across the globe may be able to damage pristine environments far from the original sources.

Over the years, several authors have applied Artificial Neural Networks (ANN) in order to predict pollutant concentration. The Multilayer Perceptron (MLP) and Elman ANN have been applied for the prediction of  $SO_2$ ,  $O_3$  and  $PM_{2.5}$  [6], [7], [8], using traffic flow and meteorological variables as input data in ANN, obtaining predictions of 1, 2 or 3 hours ahead. The results show that the ANN models performed slightly better than the deterministic and linear statistical models. Ibarra *et al.* [9] predicted hourly level for five pollutants ( $SO_2$ ,  $CO$ ,  $NO_2$ ,  $NO$  and  $O_3$ ), using MLP, Radial Basis Function (RBF) and Generalized Regression Neural Network (GRNN), obtaining that in some cases, the GRNN and RBF can perform as well or even better than MLP. The Multilayer Perceptron and linear regression have been applied for the prediction of  $PM_{10}$  in Greece [10] in five monitoring station, in your ANN model data of 24 hours and the subsequent average of the data have been used to make the final prediction. Additionally the Mixing Layer Height, the temperature, wind direction component, relative humidity are used as ANN input.

In our previous works, we have applied MLP using time window in order to perform prediction of  $SO_2$  [11] and  $PM_{10}$  [12], as well as meteorological variables. The

main problem of long time windows occurs when data is missing. In this work, we implemented a method to extract additional information about relation among pollutant and meteorological variables, in order to reduce the size of time windows and improve prediction. A MLP has been used to predict an hour ahead of pollutant concentration.

The most important issue of ANN in pollutant forecasting is generalization, which refers to their ability to produce reasonable predictions on data sets other than those used for the estimation of the model parameters [13], [14]. This issue has an important parameter that should be accounted for, it is data preparation [15]. In this work, the preparation of the data is performed by applying a clustering algorithm. Clustering involves the task of dividing data sets, which assigns the same label to members who belong to the same group, so that each group is more or less homogeneous and distinct from the others. In hard clustering (K-means), data is divided into crisp clusters, where each data set belongs to exactly one cluster. In fuzzy clustering, the data points can belong to more than one cluster, and associated with each of the points are membership grades which indicate the degree to which the data sets belong to the different clusters. For this reason the Fuzzy c-Means clustering algorithm (FCM) was used in order to find relationship among pollutant and meteorological variables. These relationship help us to get additional information that will be used for predicting. Unlike hard classification methods which force data to belong exclusively to one class, FCM allows data to belong to multiple classes with varying degrees of membership.

## II. STUDY AREA

Salamanca city is located in the state of Guanajuato, Mexico, and it has an approximate population of 234,000 inhabitants [16]. The city is 340 km northwest from Mexico City, with coordinates 20° 34' 09" North latitude, and 101° 11' 39" West longitude. The population growth, car park, industry, the refinery and thermoelectric activities, the emissions produced by agriculture, as well as orography and climatic characteristics have propitiated the increment in pollutant concentration of Sulphur Dioxide ( $SO_2$ ) and Particulate Matter less than 10 micrometers in diameter ( $PM_{10}$ ). Salamanca is ranked as one of the most polluted cities in Mexico [17]. The  $SO_2$  emissions are bigger than those emitted in the Metropolitan area of Mexico City or Guadalajara, even when these ones have a bigger population than the city of Salamanca [18].

The main causes of pollution in Salamanca are due to fixed emission sources such as Chemical Industry and Electricity Generation. The Automatic Environmental Monitoring Network (AEMN) was installed, it consists of three fixed and one mobile stations [18]. The fixed stations cover approximately 80 % of the urban area while the mobile station covers the remaining 20 %. Each station has the

necessary instrumentation to measure concentration of criteria pollutants and meteorological variables.

The measured variables are Ozone ( $O_3$ ), Sulfur Dioxide ( $SO_2$ ), Carbon Monoxide ( $CO$ ), Nitrogen Dioxide ( $NO_x$ ) and Particulate Matter less than 10 micrometer in diameter ( $PM_{10}$ ), and seven meteorological variables: Wind Direction (WD), Wind Speed (WS), Temperature (T), Relative Humidity (RH), Atmospheric Pressure (AP), Precipitation (P) and Solar Radiation (SR)[19].

The negative effects of rapid industrialization are often found in enhanced emission of undesirable and harmful pollutants. The potential role of  $SO_2$  as the largest air pollutant is well known, for it can contribute to the degradation of air quality in both spatial and temporal scales.  $SO_2$  is a colorless gas with a sharp, irritating odor. It is produced from the burning of fossil fuels (coal and oil) and the smelting of mineral ores that contain sulfur. When sulfur dioxide combines with water, it forms sulfuric acid, which is the main component of acid rain.

Acid rain forms when moisture in the air interacts with nitrogen oxide and sulfur dioxide released by factories, power plants, and motor vehicles that burn coal or oil. This interaction of gases with water vapor forms sulfuric acid and nitric acids. Eventually these chemicals fall to earth as precipitation, or acid rain. Acid rain pollutants may travel long distances, with winds carrying them thousands of miles before they fall as dew, drizzle, fog, snow or rain. When acid rain falls it can cause deforestation, acidify waterways to the detriment of aquatic life and corrode building materials and paints [20].  $SO_2$  can affect the respiratory system, the functions of the lungs and irritate eyes. When  $SO_2$  irritates the respiratory tract it causes coughing, mucus secretion, aggravates conditions such as asthma and chronic bronchitis and makes people more prone to respiratory tract infections[21].

## III. METHODOLOGY

The forecasting methodology includes the following operational steps:

- *Data preparation* for forecasting.
- *Network architecture determination.*
- *Design of network training strategy.*
- *Evaluation of forecasting results.*

### A. Data Preparation for Forecasting

The data base obtained by the AEMN, represents the essential information to be used for the determination and prediction of environmental situations. The available data set refers to a monitoring station located in a residential area of the city. Due the conditions involved in air pollutants measurements it is necessary to revise and refine the gathered

information from the AEMN. The validation of data base was done according to the INE manual [19].  $SO_2$  pollutant concentrations, Wind Direction, Wind Speed, Temperature, and Relative Humidity were used to form patterns, which were used in the implementation of clustering algorithms (K-means and FCM). The patterns were formed as follow:

$$P = [C_{SO_2}, WS, WDI, T, HR] \quad (1)$$

where  $C_{SO_2}$  is  $SO_2$  concentration,  $WS$  is wind speed,  $WDI$  is the Wind Direction Index [22],  $T$  is temperature and  $HR$  is the relative humidity. The WDI is defined according to the following expression:

$$WDI = 1 + \sin(WD + \pi/4) \quad (2)$$

### B. K-means

K-means [23] is one of the simplest unsupervised learning algorithms that solve the well known clustering problem. The procedure follows a simple and easy way to classify a given data set through a certain number of clusters (assume  $k$  clusters) fixed a priori. The main idea is to define  $k$  centroids, one for each cluster. The next step is to take each point belonging to a given data set and associate it to the nearest centroid. When no point is pending, the first step is completed and an early group is done. At this point we need to recalculate  $k$  new centroids as vary centers of the clusters resulting from the previous step. After we have these  $k$  new centroids, a new binding has to be done between the same data set points and the nearest new centroid. A loop has been generated. As a result of this loop we may notice that the  $k$  centroids change their location step by step until no more changes are done. In other words, centroids do not move any more. Finally, this algorithm aims at minimizing an objective function, in this case a squared error function. The objective function

$$J = \sum_{j=1}^k \sum_{i=1}^n \|x_i^{(i)} - c_j\|^2 \quad (3)$$

where  $\|x_i^{(i)} - c_j\|^2$  is chosen distance measure between a data point  $x_i^{(i)}$  and the cluster  $c_j$  is an indicator of the distance of the  $n$  data points from their cluster centers. The algorithm is composed of the following steps:

- Place  $k$  points into the space represented by the objects that are being clustered. These points represent initial group centroids.
- Assign each object to the group that has the closest centroid
- When all objects have been assigned, recalculate the positions of the  $k$  centroids.
- Repeat second and third steps until the centroids no longer move. This produces a separation of the objects into groups from which the metric to be minimized can be calculated.

The initial conditions for this clustering method were as follows:

- The cluster number took values from 2 to 10
- Prototypes were initialised as random values
- The maximum number of iterations was set to 100

### C. Fuzzy c-Means

The FCM was initially development by Dunn [24] and later generalised by Bezdek [25]. This algorithm is based on optimising the objective function given by the equation

$$J_{fcm}(Z, U, V) = \sum_{i=1}^c \sum_{k=1}^N (\mu_{ik})^m \|z_k - v_i\|^2 \quad (4)$$

where the matrix  $U = [\mu_{ik}] \in M_{fcm}$  is a fuzzy partition of the data set  $Z$ , and  $V = [v_1, v_2, \dots, v_c]$  is the vector of prototypes of the clusters, which are calculated according to  $D_{ikA} = \|z_k - v_i\|^2$ , it is a square inner-product distance norm.  $m \in [1, \infty]$  is a weighting exponent that determines the fuzziness of the resulting clusters.  $\mu_{ik}$  and  $v_i$  are obtained by the following equations

$$\mu_{ik} = \left( \sum_{j=1}^c \left( \frac{D_{ikA_i}}{D_{jkA_i}} \right)^{2/(m-1)} \right)^{-1} \quad (5)$$

$$v_i = \sum_{k=1}^N \mu_{ik}^m z_k / \sum_{k=1}^N \mu_{ik}^m \quad (6)$$

The optimal partition  $U^*$  of  $Z$  using the Fuzzy c-Means algorithm is reached by implementing the couple  $(U^*, V^*)$  to locally minimise the objective function  $J_{fcm}$  according to an alternating optimisation method [26].

The Fuzzy c-Means clustering algorithm was implemented to obtain the relationships between variables and get a better prediction. With the obtained result of clustering step, each pattern is labeled and this label is consider a feature.

The initial conditions for this clustering method were as follows:

- The cluster number took values from 2 to 10
- Prototypes were initialised as random values
- The number of membership degrees was set to 2
- The maximum number of iterations was set to 100
- The minimum amount of improvement was set to  $1 \times 10^{-3}$

### D. Network architecture determination

The proposed system is based on MLP. After trying with some others ANN structures, a MLP structure with two hidden layer was used. The MLP model consists of  $N$  inputs (concentration of  $SO_2$ ,  $WS$ ,  $WDI$ ,  $T$  and  $RH$ ) in time  $t = 0 \dots N$ , where  $N \in [2, 6]$ , two hidden layers of  $N$  neurons and  $N/2$  neurons respectively, obtaining as in the output the next-hour concentration. The Figure 1 shows

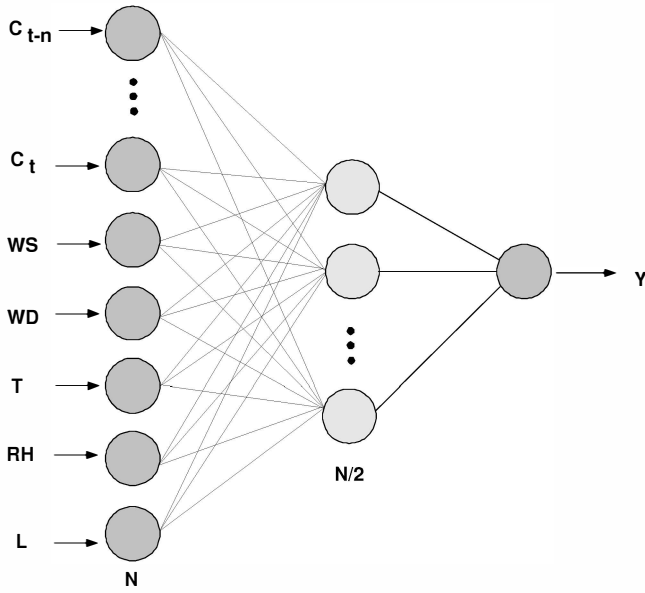


Fig. 1. Neural Network Architecture(NN-1) for 1-hour prediction.

the Neural Network architecture. The MLP with the same structure was used for all our experiments in order to find the time-window size necessary to make the best prediction using meteorological variables and labeled of clustering step.

The input patterns  $P_{in_t}$  and output patterns  $P_{ou_t}$  of neural network were formed as follow:

$$P_{in_t} = [C_t, C_{t-1}, \dots, C_{t-n}, WS_t, WDI_t, T_t, HR_t, L_t] \quad (7)$$

$$P_{ou_t} = [C_{t+1}] \quad (8)$$

where  $C$  concentration observed in time  $t$ ,  $n$  is hours before we need to make the prediction,  $L$  is the clustering label. The training set was formed with 70 % of patterns and the remaining patterns were used as test set. In addition, training and test sets were normalized in the range [0 1]. All the mathematical computations were performed using Neural Network Toolbox in Matlab©.

#### E. Design of network training strategy

The network structures used are as follows:

- Input layer:  $N$  neurons, where each neuron is feature.
- Hidden layer: one hidden layer with  $N/2$  neurons.
- Output layer: one output layer, where in the output the next-hour concentration is obtained
- Learning rate: 1
- The used activation function: the log-sigmoid function.
- Training set: 490 pattern.
- Training conditions: epoch = 200.
- Performance function: Mean Squared Error (MSE) = 0.01.

- Test set: 210 patterns.

Additionally with the best result of the prediction of an hour, five neural networks are trained to make the prediction of the next 6 hours. The Figure 2 shows the used structure, where  $P_t = P_{in_t}$  and the output of each neural network is used as input to the next network.

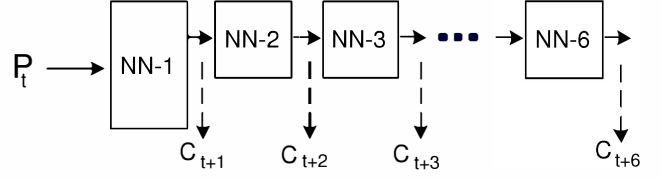


Fig. 2. Structure of Neural Networks for prediction of 1 to 6 hours.

#### F. Evaluation of forecasting results

The ANN model performance was evaluated though the following two parameters: Mean Absolute Error ( $MAE$ ), Mean Square Error ( $MSE$ ) and Root Mean Square Error ( $RMSE$ ) defined as follow:

$$MAE = \frac{1}{N} \sum_{i=1}^N |X_i - Y_i| \quad (9)$$

$$MSE = \left[ \frac{1}{N} \sum_{i=1}^N (X_i - Y_i)^2 \right] \quad (10)$$

$$RMSE = MSE^{1/2} \quad (11)$$

where  $X_i$  is the observed value at time  $i$ ,  $Y_i$  is the predicted value at time  $i$  and  $N$  is the total number of observations.

#### IV. EXPERIMENTAL RESULTS

In this work, 240 neural networks were trained. The Tables I and II show the summary of the best obtained results for each time-window with K-means and FCM clustering algorithms respectively. In each table the first column is the size time-window, second column is the number of cluster, and the remaining columns represent the prediction errors of  $SO_2$  concentrations.

The Table I shows the obtained results with K-means clustering algorithm, after creating patterns with 1 to 12 hours passed and group 2 to 10 groups. The best result was obtained with 4 hours and 2 groups, with errors in the prediction of  $MAE = 0.03280$  and  $MSE = 0.00296$ . The worst results were obtained with time-window=11 and 7 clusters, with  $MAE=0.03471$  and  $MSE=0.00338$ .

The Table II shows the obtained results with FCM clustering algorithm, after creating patterns with 1 to 12 hours passed and group 2 to 10 groups. The best result was

TABLE I  
OBTAINED RESULTS WITH K-MEANS CLUSTERING ALGORITHM

Time Window	Clusters	MAE	MSE	RMSE
1	6	0,03331	0,00300	0,05474
2	8	0,03325	0,00301	0,05490
3	4	0,03320	0,00305	0,05518
4	2	0,03280	0,00296	0,05442
5	6	0,03318	0,00298	0,05459
6	8	0,03337	0,00305	0,05523
7	6	0,03399	0,00315	0,05616
8	7	0,03414	0,00317	0,05629
9	5	0,03382	0,00311	0,05577
10	4	0,03434	0,00323	0,05680
11	7	0,03471	0,00338	0,05817
12	5	0,03543	0,00316	0,05625

TABLE II  
OBTAINED RESULTS WITH FCM CLUSTERING ALGORITHM

Time Window	Clusters	MAE	MSE	RMSE
1	5	0,03322	0,00296	0,05442
2	2	0,03305	0,00295	0,05428
3	2	0,03294	0,00296	0,05440
4	8	0,03364	0,00301	0,05484
5	3	0,03338	0,00307	0,05538
6	8	0,03353	0,00311	0,05575
7	3	0,03360	0,00313	0,05591
8	7	0,03422	0,00320	0,05657
9	3	0,03380	0,00315	0,05609
10	6	0,03449	0,00373	0,06108
11	3	0,03476	0,00409	0,06392
12	2	0,03487	0,00410	0,06569

TABLE III  
OBTAINED RESULTS FOR 1 TO 6 HOURS IN ADVANCED.

Hours	MAE	MSE	RMSE	R	d
1	0,0330	0,0029	0,05428	0.79	0.88
2	0,0458	0,0046	0,0678	0.63	0.79
3	0,0528	0,0054	0,0738	0.53	0.70
4	0,0598	0,006	0,0776	0.45	0.62
5	0,0636	0,0064	0,0801	0.38	0.54
6	0,065	0,0067	0,0817	0.33	0.49

obtained with 2 hours and 2 groups, with MAE = 0.03303 and MSE = 0.00295. The worst results were obtained with time-window=2 and 12 clusters, with MAE=0.03487 and RMSE= 0.00410.

The Figure 3 shows the best obtained result, with the FCM method using 2 hours and 2 groups. These results were used to train five Neural Networks, in order to obtain 5 hours of prediction. The table III shows the obtained results of each neural network.

In Table III, the first column indicates the hours of prediction, the following columns indicate MAE, MSE and RMSE. Additionally we estimated the coefficient of correlation (R) and the Index of Agreement (d)[27], They are shown in the last two columns. The results show that errors are cumulative, the more hours you want to predict, the error will be larger, due to accumulated prediction error of the previous hour.

## V. DISCUSSION

In a previous work [11], we had applied MLP in order to predict  $SO_2$  concentrations, where the best results were obtained with patterns formed with time-window size of three hours. Each pattern was formed with three hours of pollutant concentration and four meteorological variables (WD, WS, T, HR). In this work, we used the same meteorological variables but, we have applied two clustering algorithm (K-means and FCM) before the prediction in order to find relationship among pollutant and meteorological variables. FCM allows data to belong to multiple classes with varying degrees of membership, obtaining better results than the K-means algorithm.

The results show that using label obtained in the clustering step, it reduces the size of time window and improve pollutant prediction. In table II show that the best result was obtained with time-windows size of 2 hours and 2 clusters, with FCM clustering algorithm. The addition of clustering step reduces the size of the time-window, being especially helpful when data is missing due to errors in measurement devices.

## VI. CONCLUSIONS

In the presented work, we study the advantages of applying a soft clustering algorithm, as Fuzzy C-means, to extract information about relationship among  $SO_2$  pollutant concentration and meteorological variables (wind speed, wind direction, temperature and relative humidity) in a polluted environment prediction system. This information, plus different time-windows were tested in a MLP in order to predict an hour ahead of  $SO_2$  concentration. The best results in  $SO_2$  prediction were obtained with time-windows of 2 hours and 2 cluster, showing that it is possible to drastically reduce time window for a reasonable prediction of pollution concentration.

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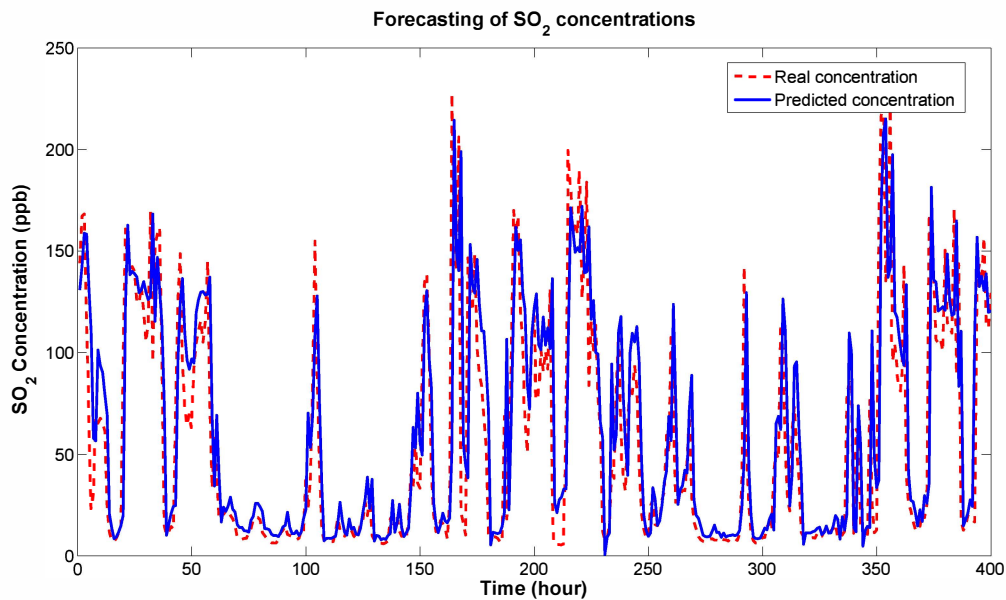


Fig. 3. Simulation Results

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